Quasinuclear Foundation for the Expansion of Quantum Mechanics

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Abstract: *The general methodology of the scientific approach [1] allows us to expand the boundaries of modern concepts. For this, as demonstrated by the example of thermoelectricity [2, 3], it is necessary to move towards expanding the phenomenology of the phenomenon, moving from primitive, noninvariant models to elementary ones, but correctly describing the phenomenon in the first approximation, and not at the expense of numerous corrections. And how to expand the boundaries of modern quantum mechanical representations shows Einstein's formulation: "Some equations of classical mechanics allow rewriting in a quantum-mechanical form" [4] - it is necessary to begin with the correction of the basic classical model.*

The Schrodinger equation is based on a primitive one-electron model of the hydrogen atom and, accordingly, is limited only by its primitive eigenvalues and radial solutions giving s, p, d, and f orbitals. The triumphant description of this model of the whole periodic table of Mendeleyev and the chemical bond [5] became the basis for its canonization into the foundation of quantum mechanics. As Nobel laureate Bob Laughlin said at a lecture in St. Petersburg: "Any quantum-mechanical problem is a solution to the Schrödinger equation" [6]. Then this equation correctly describes only one particular case. And we must pass to elementary classical models giving their eigenvalues and to make them rewrite in the operator form, and not to be limited to primitive models having similar solutions [7] on the basis of a harmonic oscillator [8].

Logarithmic relativity [3, 9] gives a general understanding of why a primitive model of a hydrogen atom is applicable to many-electron atoms - purely qualitatively it describes the energy levels of the electron shell as a whole (rather than the outer electron shell, as it is supposed). However, with an increase in the atomic number, a catastrophic quantitative divergence in the energy of the absolute values of the upper electronic levels measured experimentally and the hydrogen-like atom obtained from the model is observed [10]. In this case, the orbital of individual external electron shells obtained from the Schrodinger model do not correspond in any way to either atomic or crystalline orbitals. This, in fact, required the introduction to them of both relativistic corrections, and their hybridization.

Empirically introduced hybridized orbitals in the first approximation, poorly, and sometimes simply incorrectly describe the physical properties of crystals [11]. Starting from bare empiricism, naturally, the theory could not predict the nano-state of matter [12]. And as shown by the analysis of C & BN [13], hybridized orbitals actually substitute the first approximation of quantum mechanical solutions. A quantitative analysis of the catastrophic discrepancies between the hydrogen-like model and experimental data was carried out within the framework of a semiempiricalquasinuclear model. He showed that the description of many-electron atoms requires not only correction of hybridized orbitals, but a cardinal correction of the basic model - a transition from a primitive model of the hydrogen atom to an elementary model of a carbon atom is required. Moreover, the quasinuclear analysis performed makes it possible to refine, supplement and extend the Schrödinger model both in terms of the eigenvalues of the electron energy and in terms of bringing the symmetry of the radial solutions into correspondence with the number of external electrons.

1. INTRODUCTION

At each principal stage in the development of physics, the final element in describing the phenomenon is the equation describing the chosen model [7]. In this case, an equation that has a mathematical solution (at the time of the construction of the theory). So it was with the Langmuir equation, so it was with Maxwell's equations, so it was with the Einstein equations, so it was with the Schrodinger equation. But often in the basis of physics, at that time, existing, but not completely correct, speculative solutions are laid, which are also canonized, together with the selected models. And to describe new conjugate phenomena, such as electron emission at the nano scale, it was required to prove the rigor / limitation of the speculative solution used / received by Langmuir [14]. At the same

time, a more rigorous mathematical solution, in principle, was sufficient for an output in the description of phenomena on a fundamentally new scale. Moreover, it was enough to translate the phenomena described by Ilya Prigogine [15] from the category of "forbidden" to the category of allowed [16].

Similar "non-rigor" lies in the foundations of quantum mechanics: a primitive model of the hydrogen atom is used and has, at the time of its formation, a mathematical solution, a primitive equation for the eigenvalues (eigenfrequencies) of a harmonic oscillator. This is what leads to the fact that they turn a blind eye to the many contradictions arising in the quantum-mechanical description, contradictions with "common sense", that is, with a classical description. So, for example, on the maximum probability density of the electron orbital at the center of the nucleus.

Apparently, this is the reason for the "misunderstanding" of quantum mechanics and the Nobel Prize winning for the quantum photoelectric effect by Einstein [4], and only in attempts to "understand" it not halted in conventional notions by Mandelstam [7], and in the attempts to rewrite quantum mechanics [17]], and in attempts to reinterpret the wave function [18]. This is the reason for using numerous approximations, which are necessary even for a qualitative agreement between the results of quantum mechanical calculations and experiment.

All this indicates that in its fundamentals lies not a complete and not orthogonal frame. As Richard Feynman said: "We scratch the right ear with the left hand." Therefore, for modern quantum mechanics, the solution of the three-body problem (father and son Fadeev) is associated with colossal mathematical difficulties, whereas it was shown in [13] for the description of electronic orbitals in the first approximation, in the elementary model it is necessary to repulse not from the primitive hydrogen atom, but rather to use elementary carbon atom.

But before proceeding with the construction of the model and the calculation of the electron orbitals, correctly in the first approximation describing the orbitals of C & BN, before tackling the necessary refinement of the Schrödinger equation, we will try to construct a semiempiricalquasinuclear model that will allow us to draw a rough but general picture. This model is compilative, because it itself repels itself from analysis within the framework of generally accepted orbitals of the hydrogen-like atom. But this model allowed to systematize and quantitatively analyze the discrepancy between the model of the hydrogen atom and the experimental data. Thus, she focused on the fundamental inaccuracies in the generally accepted calculations of atomic orbitals lying in the foundations of quantum mechanics.

A coherent, cross-cutting and more detailed presentation of the presented part of the work will be done in the book. In the same communication, it was necessary to include some already published fragments for readability / understanding (without constant peeking in previous articles).

2. THE BEGINNING OF QUASINUCLEAR ANALYSIS OF ATOMIC ORBITALS

With an increase in the atomic number, a catastrophic divergence in the energy of the absolute values of the upper electronic levels measured experimentally and the hydrogen-like atom obtained from the model is observed [9] (Fig. 1).
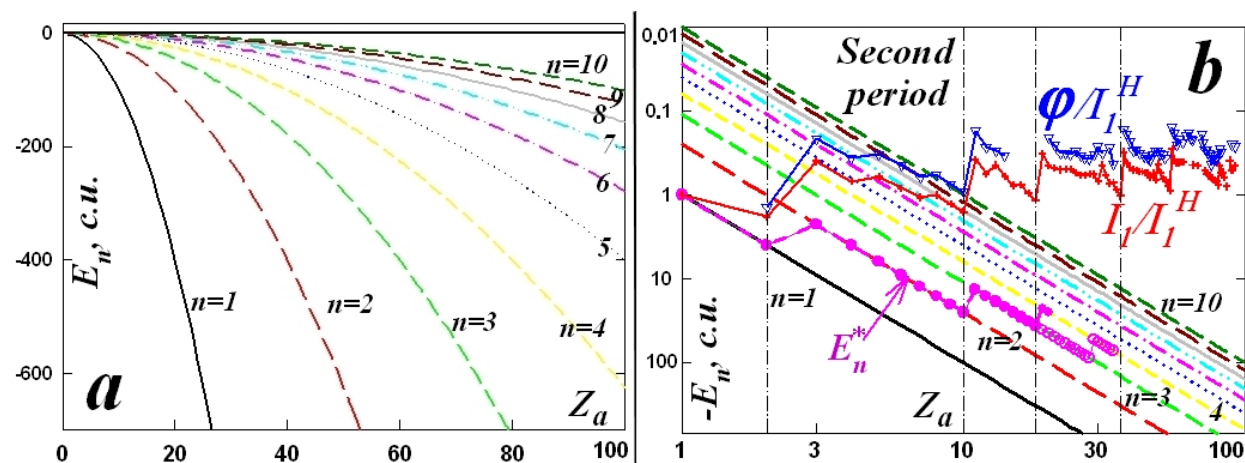
Fig.1. Dependence of the energy of allowed electronic levels (in conventional units) on the atomic number in linear (a) and double logarithmic scale (b). Pink dots show the maximum filled levels (within the framework of the elementary model). Red crosses and blue triangles show normalized reference data on the first ionization potential I_1 / I_1^H and the work function φ / I_1^H.

As can be seen from Fig. 1b, this catastrophic discrepancy has a natural character, it grows with the increase in the atomic number. This regular discrepancy indicates that the use of the potential energy of an electron relative to a bare nucleus in the Schrödinger equation is incorrect for describing the external electron orbitals of many-electron atoms.

To construct a quasinuclear model, we use the fact that the model of hydrogen-like atoms correctly describes the very occurrence of periodicity-it gives atomic numbers of the end of the periods for chemical elements. True, as can be seen from the third period (Fig. 1b), it is not always unambiguous (to explain the ambiguity, the assumption is used about the different rates of "ascent" of the shells). And the ionization potentials of inert gases do not increase with the increase in their atomic number, as should follow from the Schrodinger model, but remain at approximately the same level of energy and even decrease somewhat.

Nevertheless, the change in the ionization potentials within the periods qualitatively corresponds to the filling of the s, p, and d levels of the hydrogen-like model. Therefore, if for each period we take our reference point - our zero "starter" charge of the shielded core of the corresponding inert gas, the addition of an additional proton will give an excess charge field acting on external electrons.

And so, initially we will assume that inert gases are quasi-periods. The "screening" of the nucleus by their completely filled electron shells is manifested in an experiment in the reduction of the hydrogen-like charge of even helium. And the effective charge of quasinasters can be calculated using formula 1

$$E_n = -\frac{hcRZ^2}{n^2} \Leftrightarrow -\frac{hcRZ^{*2}}{n^2} = E_n^{Exp} \tag{1}$$

For the quasinuclear model of a hydrogen-like atom, the screening coefficient of the hydrogen nucleus itself is naturally set equal to unity. Here the coefficients of the screening of the nuclei by the inner shells k^Z are obtained from the formula 2

$$k^Z = \frac{Z^*}{Z} = \sqrt{\frac{E_n^*}{E_n}} \tag{2}$$

Thus, the nuclear potential is modified, which determines (in the Schrodinger equation) the allowed energy levels of the external electrons and reduces them in absolute value, bringing them into better agreement with the experiment.

Using the data presented in Fig. 1, we first obtain the screening coefficient for the nuclei of the first three inert gases, which are presented in Table 1

Table1.

noblegas	He	Ne	Ar	…
k^Z	0.6723	0.2519	0.1724	

Similarly, all subsequent shielding ratios of inert gases can be obtained. But the "natural" growth of the screening of the core with the increase (size) of the filled shell is already visible from the table given, which seems to be in favor of the assumption made.

The size of the quasinuclear is determined by the orbits of the inner electron shells, which is also manifested in effective screening. In this case, for the subsequent elements of the second period (as for other periods), there are two ways of calculating the energy levels.

The first, rather conditional way: the atom's quasi-nucleus "has" a charge equal to the number of external electrons (no matter how "proton" superfluous for a quasinuclearare not screened). This unnatural path also gives an unnatural alternation of identical fillings of hydrogen-like orbitals for each period.

The second, more natural way is to take into account the screening coefficients of the quasi-frame of the given period given in Table 1 for all elements of a given period.

However, the empirical through-dependence of the quasinuclear "shielding" coefficient on the atomic number for the first periods shows (Fig. 2), what:

firstly, the relatively slightly changing "screening" coefficient for the entire period should be determined not by its value for the corresponding inert gas (red circles in Fig. 2), but by the following element having one external electron (black crosses in Fig. 2),

secondly, a nonmonotonic change in the "screening" coefficient within the periods indicates a transformation of external orbitals that is not taken into account by the hydrogen-like model when another electron is added. Those. Ala-hybridization of Pauling occurs already at the atomic level and real atomic orbitals are not described by hydrogen-like s-, p-, d-orbitals. So, strictly speaking, s-, p-, d-orbitals describe excited states of only a hydrogen atom.

The increase in the size of quasinuclear should also be taken into account when constructing true orbitals. As well as the features noted above, leading to a nonmonotonic dependence of the first ionization potential within the periods. But this paragraph is not accidentally called "beginning", tk. the obtained estimates of the screening coefficient of the nuclei only modify the model of the hydrogen-like atom-they adjust the basic parameter in the first approximation to the experiment.
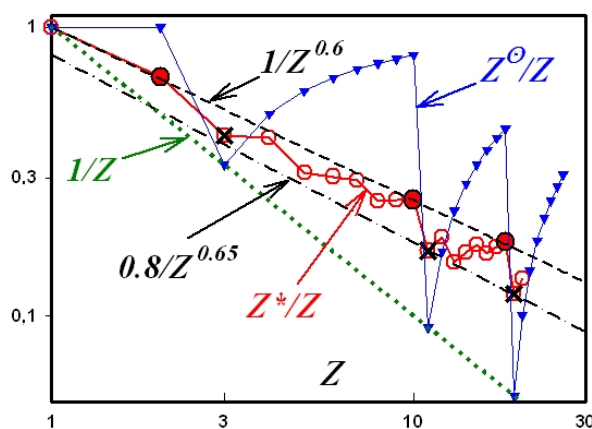

Fig.2. The end-to-end dependence of the coefficient of quasinuclear "screening" on the atomic number: large filled circles show the coefficients of (self) "shielding" of inert gases (short dash), crosses show the actual coefficients of "shielding" of the outer electrons of the corresponding period (dash-dot) filled with envelopes of inert gases, blue triangles - the screening coefficient for a complete subtraction of the charge of the corresponding electron shell of an inert gas (according to formula 2), green dots - screening of the last electron all electrons below.

And since purely electrostatic shielding by internal electron shells does not give any additional attenuation (and the helium atom simply does not have them), the first conclusion is that the hydrogen-like model quantitatively gives the allowed energy levels correctly only for the hydrogen atom.

Quasinuclear model, as already noted, is simply a compilation (carried out to analyze / systematize the principal differences between the energy levels allowed by the theory and those observed experimentally). Nevertheless, already this compilation shows that in the original classical equation (in the Lagrangian used in the construction of the Schrödinger equation), a modification of the nuclear charge entering through the potential energy and, accordingly, a modification of the solution of the Schrödinger equation is required. In this case, the formula 1 is transformed into the formula 2:

$$Z^{\square} = Z - Z^{noble\ gas} \Rightarrow E_n = -\frac{hcR(Z^{\square})^2}{n^2} \tag{3}$$

where $Z^{\square}$ - the charge of the external electron shell.

But from the comparison of the shielding coefficient only by the filled electronic shells (blue triangles in Fig. 2) with the experimental screen screening coefficient (red circles in Fig. 2), it is clear that this formula also gives a large discrepancy with the through experimental screening coefficient. In the given graph $Z^{\square}/Z$, a substantial, even superfluous screening, filled with a shell for one, the first external electron, is visible. But fully filled electronic shells do not completely compensate for the

corresponding portion of the nuclear charge for two or more external electrons. screening of fully filled shells is manifested only in the form of a small increase in its strength against the background of screening by any, including external, underlying electrons.

Thus, if we stay within the framework of a primitive hydrogen-like model of the atom, then in this rough approximation the quasinuclear model allows us to correct the allowed energy levels of the last electron

$$z^* \square z^{0.4} \Rightarrow E_n \square -\frac{hcRZ^{0.8}}{n^2} + \delta$$

(4)

where δ - a small correction. But in addition to taking into account the quasinuclear of such a "hydrogen", it is necessary to take into account all preceding external electrons. But to take into account the influence of external electrons, one already needs to take into account the geometry of their orbitals.

When analyzing the physical properties of C & BN [13], it was shown that, in addition to energy divergences, the shape of the external orbitals of the hydrogen-like model does not correspond to the spatial symmetry and properties of these materials. The introduction of nuclear hybridization (relativistic corrections) or crystalline (Pauling hybridization) to a hydrogen-like model was made by "corrections" that attempted to restore the conformance of the shape of the orbitals to the physical properties of materials.

However, "corrections" were introduced that were superior to the basic terms of the hydrogen-like model both for the energy levels of the electrons and for the spatial distribution of their density around the nucleus. Those.and this actually substitution of atomic orbitals did not bring the theoretical calculations in the first approximation in accordance with the experiment. Thus, the hybridization introduced by Pauling itself gave a catastrophic discrepancy with the experiment on the binding energy between monoatomic layers from hexagons in C & BN, which was the starting point of this analysis [11].

As was shown in [9, 12], the symmetry of external orbitals is determined by the number of external electrons. So, strictly speaking, the very s-p-d-f-classification of electron shells of a monatomic shell also requires refinement when used. Natural just by symmetry for a single electron neutral, not exposed to any action of the hydrogen atom, finding an electron on both sides of the nucleus becomes unnatural with an increase in the number of external electrons, which is shown in the example of C or BN orbitals (Fig. 3).

Thus, as a quasi-nucleus, it is necessary to consider the nucleus together with the filled electron shells (inert gases), but the use of the hydrogen-like model is valid only for atoms with one external electron.
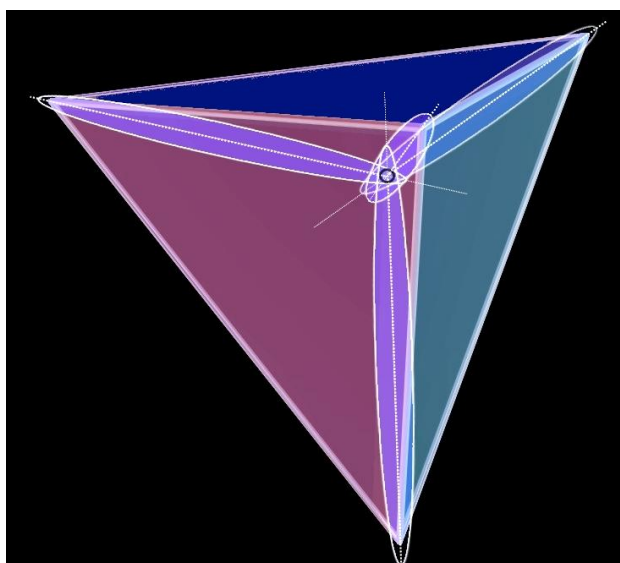

Fig3. *Orientation of the true atomic orbitals of C & BN to the vertices of the tetrahedron*

3. ELECTRON IN ASYMMETRIC POTENTIAL

Elementary, but not primitive as a hydrogen atom, a carbon atom, makes it possible to use both the concept of a quasi-nucleus and take into account the influence of all external electrons on each of them. Therefore, we use the quasinuclear model of a carbon atom as a base model and determine the basic stationary state of each electron in the form of a solution of the electrostatic problem for their "centers of gravity." To solve this problem, we use the symmetry of a regular tetrahedron obtained for carbon atomic orbitals. In order to find stationary solutions for each electron on the "tetrahedral" orbit, one can introduce one and the same deformation of the quasinuclear potential due to the electrostatic fields of the "centers of gravity" of the remaining three electrons (Fig. 4).
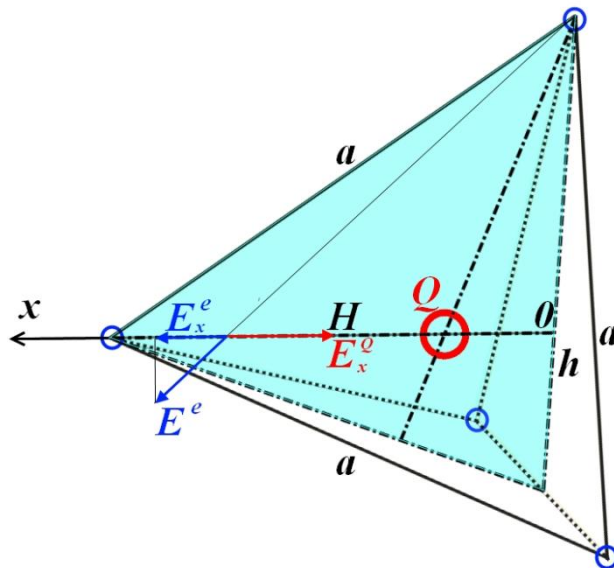

Fig4. *Calculation of the electric field E_x^{-e} strength along the volume symmetry axis of the tetrahedron H for the repulsive (right) electron and for quasi-nucleus Q located in the tetrahedroncenter.*

The sum of the fields of all these four electrons in the center of the tetrahedron, due to symmetry, is zero. The vector sum of the electric fields of three (repulsive) electrons is directed along the volume bisector / height of the tetrahedron. So, to solve the above problem, the total field of each external electron can be replaced by its projection on the bisector / height of the tetrahedron. In this case, each extracted electron is in the total potential of the quasinuclear and the remaining three electrons.

Thus, to solve the corrected quantum mechanical problem, it is sufficient to solve the one-dimensional problem-to determine the distribution along the tetrahedron axis of the potential of the quasinuclear and the potential of three electrons located at the vertices of the tetrahedron on the repelling face (on the right).

For repelling the selected (trial) electron of three other electrons, the problem can also be simplified: using an elementary geometric calculation, determine the projection on the x-axis of the strength of the electric field of one electron and multiply it by 3, starting from the symmetry of the tetrahedron.

Assuming the edge of the tetrahedron and the physical constants equal to unity, we obtain expressions for the electric fields acting on the electron located on the left in Fig. 4:

$$3\mathrm{E}_x^{-e} \square \frac{3}{\left(1+\frac{1}{3x^2}\right)^{3/2} x^2} \quad , \quad \mathrm{E}_x^Q \square -\frac{Q/e}{x^2\left[1-\frac{1}{2\sqrt{6}x}\right]^2} \tag{5}$$

Naturally, when the total electric field of all four electrons in the center of the quasinuclear set is equal to zero, it is strictly satisfied also for the calculated projections

$$\left|3\mathrm{E}_{x_Q}^{-e}\right| = \left|\mathrm{E}_{H-x_Q}^{-e}\right| = \frac{8}{3} \tag{6}$$

And for an arbitrary value of the coordinate along the volume axis of the tetrahedron, the calculated projections of the electric fields (formula 4) are shown in Fig.5.
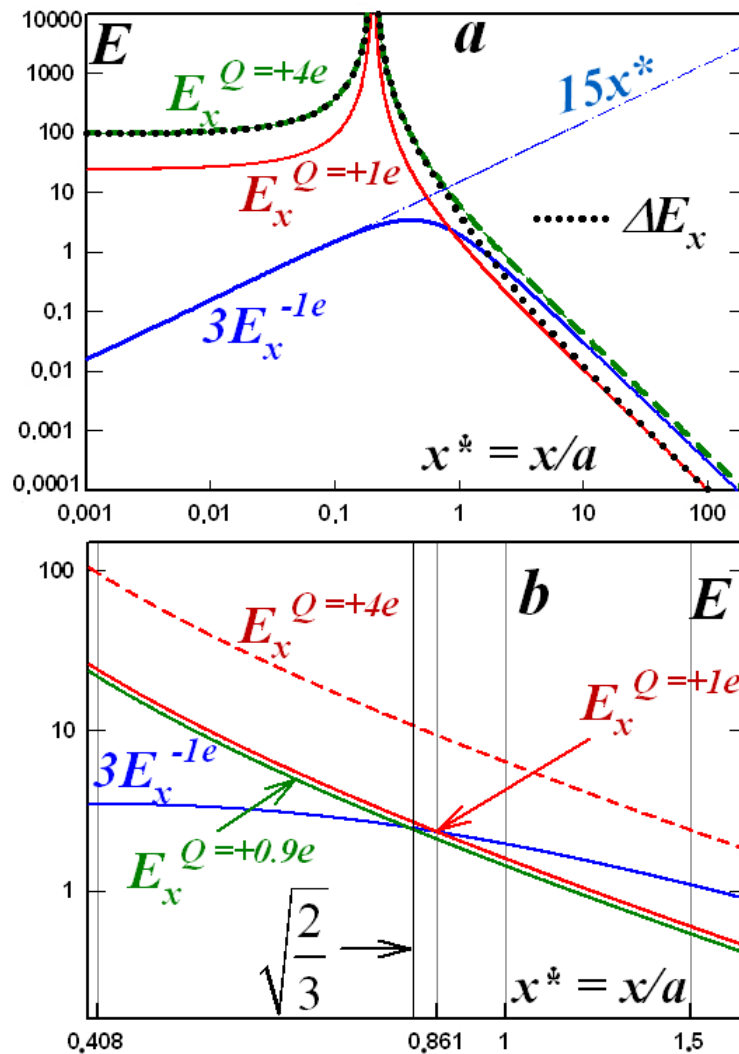
Fig5. *Distributions of the electric field projections onto the volume axis of the tetrahedron*

As can be seen from Fig. 5, if the charge of the quasinuclear is put equal to the total number of external electrons: $Q= +4e$, then the absolute electric field of the repulsive three electrons $3E_x^{-e}$ located at the vertices of the tetrahedron is always less than the attracting electric field of the quasi-nucleus $E_x^{Q=+4e}$, which is quite natural, tk. the quasi-frame is located and closer to the probe, the displaced fourth electron and has a larger charge than the repulsive face of the tetrahedron with three electrons.

In addition, the projections E_x^{-e} tend to zero inside the tetrahedron and, as a consequence, and ΔE_x -the difference of the fields $3E_x^{-e}$ and $E_x^{Q=+4e}$, tends to the field of the quasi-frame $E_x^{Q=+4e}$. For points outside the tetrahedron at large distances, the electric field for the ionized atom (in contrast to the neutral one) is naturally conserved and, as shown by the difference in the intensity ΔE_x from the black points in Fig. 5, the total electric field of the ion outside the tetrahedron passes into the Coulomb field of one positive charge, which should occur for a single ionized atom.

It is typical for the transition region that, as can be seen from Fig. 5b, near the coordinate of the vertex of the tetrahedron: $x = \sqrt{\frac{2}{3}}$, the repulsive force of the trial electron $3E_x^{-e}$ is completely balanced by the attraction force of the ion $E_x^{Q=+1e}$. But this is an unstable equilibrium against the background of the Coulomb force $E_x^{Q=+3e}$, which is giant in the neighborhood of the vertex of the tetrahedron.

Integrating the electric fields shown in Fig. 5, we obtain the corresponding electrostatic potentials:

$$\varphi_x^{-3e} = \text{Abs}\left[\frac{3\sqrt{3}}{\sqrt{3 + \frac{1}{x^2}}\, x}\right], \qquad \varphi_x^{+Q/e} = \frac{Q}{e}\text{Abs}\left[\frac{12}{\sqrt{6} - 12\, x}\right]$$

Integrating ΔE_x, we obtain an asymmetric spatial dependence of the real electrostatic potential in which the emitted electron is located (Fig. 6)and which, naturally, differs from the simple, symmetric Coulomb potential of the charge of the nucleus, which is put into the one-electron Schrödinger equation
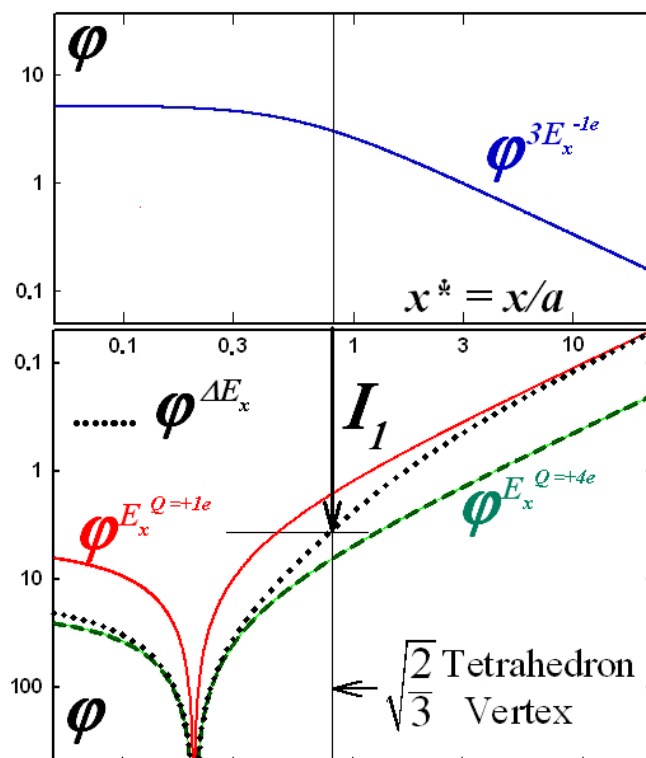

Fig6. *The distribution of the electrostatic potential along the tetrahedron axis: from below*

symmetrical Coulomb potential of the quasinuclear without taking into account the repulsion of three electrons on the opposite face of the tetrahedron (green dotted curve), the asymmetric potential of the quasinear with allowance for the repulse of the test charge (a dotted black curve) and the symmetric Coulomb potential of the ion (red curve), on top - the repulsive potential of three electrons on the vertex tetrahedron, opposite to the isolated probe fourth electron.

The asymmetric dependence of the electrostatic potential shown in Fig. 6 shows that for the appearance of the electrostatic equilibrium state of an electron at the vertex of a tetrahedron, repelling one external electron by three others is not enough. But the very fact of the existence of an equilibrium state of an electron at the apex of a tetrahedron indicates that there exist short-range repulsive forces from the quasinuclear. The catastrophic decline of these repulsive forces at large distances outside the tetrahedron, the distribution of the total potential changes insignificantly.

This makes it possible to determine with good accuracy the first ionization potential I_1 from the right wing of the resulting asymmetric dependence of the potential. As is clearly seen from the figure, it is substantially larger than the ionization potential of a single charged ion and is substantially smaller than the potential obtained from taking into account the total charge of the quasinuclear. Especially I_1 is less than the potential obtained from taking into account the total nuclear charge that enters the Schrödinger equation when calculating allowed electron states, which leads to a catastrophic discrepancy between the experimental data and the one-electron model applied to the many-electron atoms.

In this case, taking into account the fact that the equilibrium of the attractive force of a single-ionized atom and the repulsive force by three electrons shown in Fig. 5b is not accidental near the vertex of the tetrahedron, the resulting asymmetric dependence of the total potential can be decomposed into the symmetrical and asymmetric components: shown in Fig. 7.

$$\varphi^{\Delta E_x} = \varphi^{E_x^{Q=+4e}} - \varphi^{3E^{-1e}} \equiv \varphi^{E_x^{Q=+3e}} + \{\varphi^{E_x^{Q=+1e}} - \varphi^{3E^{-1e}}\}$$
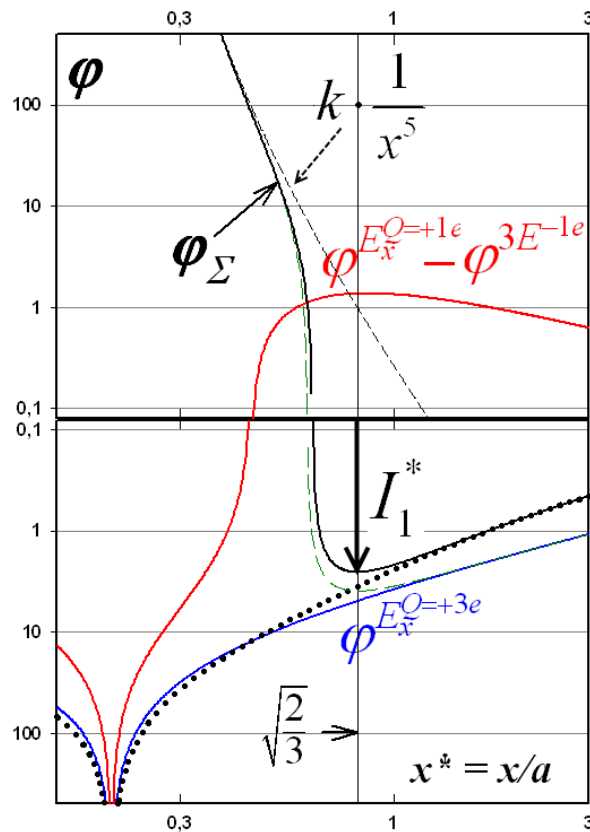
(7)

Fig7. *The spatial distribution of the total potential and its components along the tetrahedron axis: the upper part of the figure corresponds to the potentials repelling the electron, the lower one to the attracting potential.*

In calculations of many-electron atoms, only the symmetric Coulomb component is used in the one-electron Schrödinger model, and even then for the total number of electrons, and the asymmetric component is not taken into account at all. In the framework of such a very crude, but analytical solution of the Schrödinger model, the repulsion of an electron from the nucleus is described at the expense of an elementary oscillator, after the operator rewriting its equation. This dynamic "repulsion" is associated with the electron orbit at the upper stationary level, the catastrophic divergence of which with the experiment was shown above.

Не касаясь природы сил отталкивания, просто учтём этот хорошо известный эмпирическийфенологический факт - такие силы малого радиуса действия существуют. Оптимизируя степень и сомножитель их потенциала $k \cdot \frac{1}{x^5}$ так, чтобы полный симметричный потенциал $\varphi^{E_x^{Q=+3e}} + k \cdot \frac{1}{x}$ не нарушал равновесия на вершине тетраэдра (производная равна нулю), мы получим, прибавив ассиметричную компоненту потенциала, изображённый на рис.7 суммарный потенциал φ_Σ - потенциальную яму, дно которой определяет стационарное состояние электрона и скорректированное значение первого ионизационного потенциала I_1^*.

Without touching the nature of the repulsion forces, we simply take into account this well-known empirical phenological fact - such short-range forces exist. Optimizing the degree and the factor of their potential $k \cdot \frac{1}{x^5}$ so that the total symmetric potential $\varphi^{E_x^{Q=+3e}} + k \cdot \frac{1}{x}$ does not violate the equilibrium at the vertex of the tetrahedron (the derivative is zero), we obtain by adding the asymmetric component of the potential, the total potential φ_Σ represented in Fig. 7, - the potential well whose bottom defines the stationary state of the electron and the corrected value of the first ionization potential I_1^*.

4. CONCLUSION

The analysis has shown that for an individual atom, there is a need to find / choose (almost as did Pauling) the true quasinuclear, initially "hybridized" orbitals of the atom itself (as 4 external electron orbitals for C & BN were chosen).

But for a rigorous calculation of atomic orbitals, of course, the Schrodinger equation is not sufficient. Perhaps Einstein's phrase: "Some equations of classical mechanics allow rewriting in a quantum mechanical form" should be understood not simply as an acknowledgment of the Schrödinger equation, but broader and a new equation must be sought, the rewriting of which will give an overall picture, rather than a special case, hydrogen. And when a fundamentally new operator method was used, the model of a hydrogen-like atom reduced all of the quantum mechanics to a particular case.

This requires the expansion of quantum mechanics itself.

First, a modification of the calculation of the eigenvalues of energy-allowed levels is required, which has so far been done only within the framework of the empirical quasinuclear model.

Secondly, it is required to find additional radial solutions (wave functions) whose symmetry corresponds to the number of external electrons, and not to a single one, as in the calculation of a quasi-hydrogen-like atom. In this plan, instead of the primitive orbitals of the hydrogen-like atom, elementary orbitals obtained in papers on C & BN can be used.

But, strictly speaking, to find stationary orbitals it is not enough and to be limited only by the proper solutions of only a primitive harmonic oscillator; by definition, it gives only oscillations, i.e. stable excitations-vibrations of electronic orbitals. And to find the basic states of electronic orbits, we will have to return to the search for more correct classical models and apply the operator method to them.

And so, the semiempirical model of the quasinear allowed not only to systematize the observed catastrophic differences in the calculations within the one-electron atomic mode, but also revealed the phenomenological omissions in the application of this model to many-electron atoms. And since the axiomatics of quantum mechanics itself is also built on the basis of a one-electron model: the seemingly general approach based on Lagrangians and Hamiltonians was in fact used to describe a particular case. Then the analysis shows the way of expansion of quantum mechanics - it is necessary to search for classical models in a first approximation, describing the phenomenon under investigation and re-writing the equations obtained in the framework of these models in the operator form. At the first stage of the expansion of the quantum-mechanical description of both atoms and solids, it is possible to replace the Coulomb potential by the resulting total potential φ_{Σ} in the Schrödinger equation.

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